Benchmark testing of Th-232 ACE file

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Problem: Incorrect multiplicity flag in the TYR block of the ACE file
(identified by Marieke Duivestijn)

Tests

1. Convert MF6 to MF4/5 representation

2. Manually change the multiplicity flag in the TYR block

3. Prepare updates for ACER of NJOY

4. Analyse the effects on benchmarks

Results

1. MF4/5 representation

The SIXTAB code was used to convert MF6/MT18 block into comparable MF4/MF5 representation. An error in the interpolation table of the resulting files was corrected manually. Two cases were considered when generating ACE files:

a. Angular distributions were forced isotropic.
b. Anisotropy was included in file MF4.

The calculated multiplication factor for the KBR lattices was unreasonable when anisotropy was included. A test was made by manually changing the flag in the TYR block from -19 to +19. The results became very similar to the isotropic case.

2. Change of multiplicity flag in the TYR block

The ACE file generated from the fission spectra in MF6 representation was edited manually, changing the multiplicity flag in the TYR block form -1 to +19. The results

agreed in all cases with those from item 1.b. above to within the statistical uncertainties. If the flag was set negative, the calculated values of the multiplication factor were about 1000 pcm higher, as in the case with MF4/MF5 data representation.

3. Updates for ACER of NJOY

Conclusions from the above test are:

- NJOY produces ACE files with incorrect multiplicity flag when fission spectra are given in MF6 representation (consistent with the observation of M. Duivestijn).
- MCNP does not like the CM flag for fission spectra.

A patch labelled "upiaea13" is proposed to fix processing of ENDF files with fission spectra in MF6 representation.

4. Benchmarks

Benchmarks from the International Criticality Safety Benchmark Experiments were considered, namely Thor (PU-MET-FAST-008), KBRnn (IEU-COMP-FAST-002, IEU-COMP-INTER-001, IEU-COMP-THERM-005, HEU-MET-FAST-068, HEU-MET-INTER-008) and SB-n (HEU-COMP-THERM-015, U233-COMP-THERM-001). Since the calculations with "pure" ENDF/B-VII library could not be performed, only the results referring to changes due to different versions of the Th-232 ACE file are relevant. Differences are given in pcm. "Dif.TYR" is the difference due to the correction of the yield flag in the TYR block relative to the uncorrected ACE file. "Dif.MF5" is the difference between corrected files geneated from MF6 and MF4/MF5 representation, respectively. The uncertainty in the differences (in braces) is the sum of the statistical uncertainties in the calculations.

Benchmark	Dif.TYR	Dif.MF5
Thor	-110(8)	-7(8)
KBR22	-333(104)	-57(106)
KBR23	-161(119)	-126(119)
KBR18	-568(60)	-47(60)
KBR19	-548(80)	-78(78)
KBR20	-264(106)	-103(104)
KBR21	-159(113)	+28(113)
SB-1	+125(20)	+22(19)
SB-5	+63(18)	-2(18)
SB-2	+168(22)	+41(22)
SB-1+1/2	not available	
SB-3	not available	
SB-4	not available	
SB-6	+56(20)	+52(20)
SB-7	not available	

The IPPE benchmark on the leakage spectrum from ^{232}Th sphere with a D-T source was also analysed. Some comments on the benchmark were reported in the INDC(NDS)-0493 report, which is available electronically from "http://www-nds.iaea.org/indc_sel.html". The spectra are compared in Figure 1.

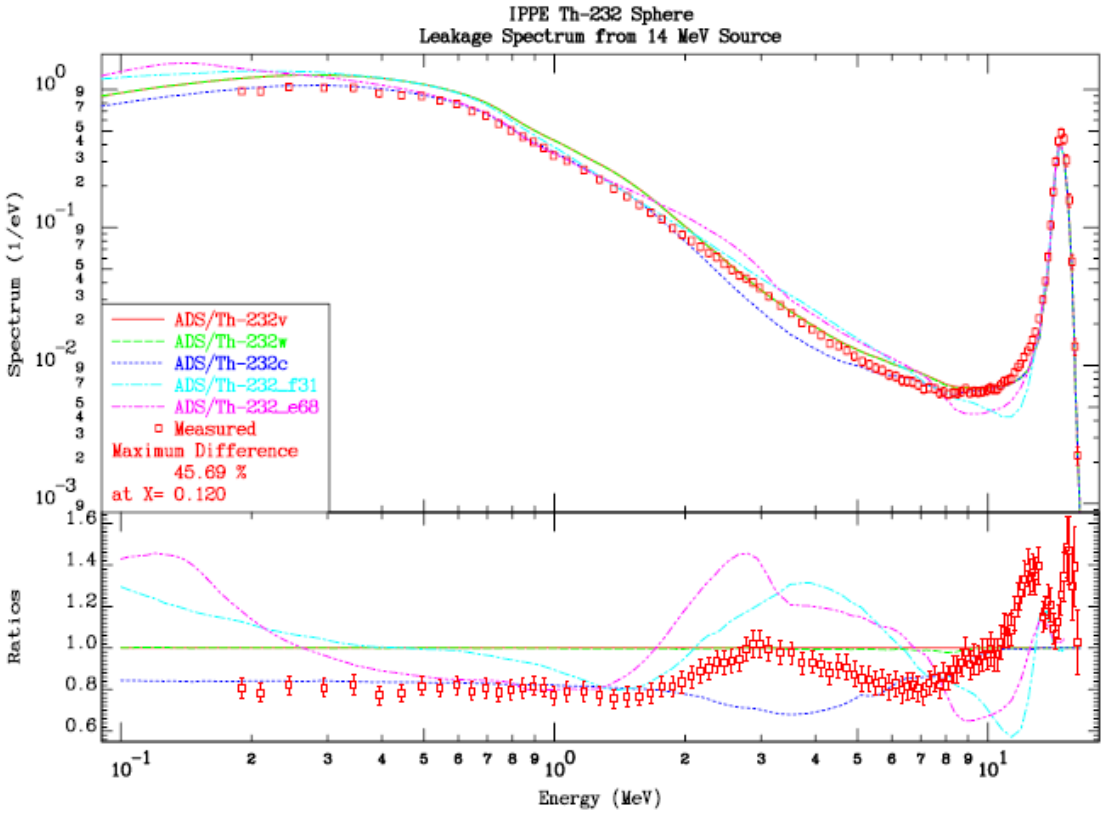

Figure 1: Leakage spectrum from the IPPE Th sphere with D-T source. Suffix in labels implies: v – corrected ACE file, w – ACE file generated from fission spectrum data in MF4/MF5 representation; c – uncorrected ACE file; f32 – JEFF-3.1 data for ^{232}Th; e68 – ENDF/B-VI.8 data for ^{232}Th.

The main conclusions are:

- Spectra with MF4/MF5 representation (suffix w) are practically the same as those generated from the spectra in MF6 representation (suffix v).
- The spectra with corrected flag in the TYR block agree with measurements better than with the uncorrected file (suffix c) in the 2-6 MeV range, but are systematically higher by 20% at lower energies.

Conclusions

- ACER of NJOY99.112 produces incorrect ACE files when fission spectra are given in MF6 representation.

- MCNP requires fission spectra in the LAB coordinate system. Since fission is applicable only to the actinides, the difference is not significant.

- A patch for NJOY is proposed that enters the correct yield flag (+19) into the TYR block of an ACE file.

- The patch was verified by converting MF6 data into comparable MF4/MF5 representation and generating an alternative ACE file. Benchmark results with the two files agreed to within the statistical uncertainty in the calculations.

- The impact of the error in the ACE files is small for thermal lattices.

- The correction for ACER results in a REDUCTION of the multiplication factor in a thorium-reflected fast lattice Thor by about 100 pcm.

- The KBR lattices are particularly sensitive to thorium data. The correction results in a REDUCTION of the multiplication factor in the lattice with the hardest spectrum by as much as 500 pcm. Lattices with a softer spectrum are less affected.

- Leakage spectrum from the IPPE thorium sphere with D-T source is strongly affected. The hole in the spectrum from 2-6 MeV disappears, but at lower energies the spectrum is now systematically overpredicted by 20%.

Patch for ACER of NJOY

```
*ident upiaea13
*/ acer -- 05jun06
*/  set nu-bar for neutron multiplicity on MF6 fission (trkov, iaea).
*/  force lab coordinate system.
*/  (Th-232 from ENDF/B-VII with anisotropic fission neutron
*/  distributions)
*/  exclude redundat lumped cross sections mt 851-870, if present.
*/  (not allowed by ENDF rules but needed by ERRORR).
*d acer.5401
c               set flag for CM system, except fission
              if (lct.ge.2 .and. mth.ne.18) n=-n
*i acer.6432
         if(mth.eq.18) ntyr=19
c          force lab coordinate system for fission
         if(mth.eq.18) lct=1
*i acer.1938
     &           (iverf.ge.6.and.(mt.ge.851.and.mt.le.870)).or.
```